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Calculations of Wind Mass Transfer of Pollution: Simulation and Analytical Models

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Abstract: The main goal of the present study is to compare the results of calculations of the dust mass transfer with wind using the analytical and simulation models. Analytical model is based on unsteady turbulent diffusion equation. Simulation model is taking into account four main processes of mass transfer in atmosphere: emission of pollutants, wind mass transfer, deposition and turbulent diffusion of pollutants. Calculations of pollution field from linear source were compared. It was found that both results are in good agreement. Some special features of the simulation model make it more preferable for pollution forecast calculations for the purposes of optimal environmental management.

Keywords: Management and Environmental Science, Numerical Methods for Optimization, Air Pollution, Cellular Automata.

1. INTRODUCTION

Management in the field of environmental protection is based on information not only about the actual levels of the pollution, but their values and forecasts in the future. The latter is a non-trivial task, since the formation of fields of surface contamination is the result of many anthropogenic and natural factors. Wind mass transfer polluting substances (from the emission source to the place of deposition) generates a field of surface contamination, the secondary mass transfer (including wind) has on them a significant additional effect: blurs the boundary and change the shape of fields, concentrating pollution in some areas contaminated territory, at the same time reducing the concentration of harmful substances on others. The action of secondary mass transfer may take years and be local (e.g., diffusion of the pollution in the surface layer of the soil), but may be short enough and comparable in scale to a primary area of contamination. The most vivid example of the action of the wind mass transfer is the formation of the field of radioactive contamination in the Urals in the middle of the XX century. When the wind from the shores of Lake Karachai raised dust of radioactive waste and scattered in an area of tens of square kilometres.

Traditionally, the mathematical model of wind mass transfer is recorded analytically in terms of differential equations. At all usability of the developed apparatus for solving them, at the stage of task developing (making the equation or their system) are frequently encountered significant difficulties associated with the need of taking in account the nontrivial boundary conditions (e.g., complex inhomogeneous relief of the underlying surface), actions related to mass transfer of physical and chemical processes in an atmosphere with contaminants and other factors. Estimated distribution of pollution produced by such models is average and has a smooth character, which is not always observed in reality (Chukanov 2006). In such a situation, it is advisable to go to a simulation that takes into account the probabilistic nature of the formation of each particular field of pollution.

Simulation models in the computing environment of cellular automata (CA) (Toffoli, Margolus 1991) are an alternative to differential equations in modeling of complex physical processes. CA model worked well in various physical applications and allow relatively easy to implement superposition of sources of various shapes and intensities, as well as the multiplicative effect of nonstationary stochastic emissions and meteorological processes.

The mail goal of the present study is to compare the results of calculations of the dust mass transfer by wind using the analytical and simulation models. As a tool for simulation, there was chosen the "Universal CA Laboratory PyCALab" (Berg 2005) developed in the language of Python (Beklemishev 2006).

2. THE WIND MASS TRANSFER

It is known that a solid particle under the influence of wind can slide, roll and lift off the surface, Fig. 1. Rolling and sliding particles interacting with a surface roughness in the end may be disturbed in the surface wind field, where, under the influence of random fluctuations of wind, may go even higher and get into the area where the main contribution to

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the transfer of particles makes wind transport. The particles of relatively "big" masses cannot rise high above the surface, and so they make saltation movements, that is to say simply bounce and thus move from one place to another. It is proved that flipping processes are dominant at sandstorms, under the influence of this process is transferred to 75% of all particles. Here we review the wind transport of particles to rise above the surface as a result of various factors (location of the source of emission of pollutants above the ground, the wind capture low dispersing dust from the surface of the source of contamination), flipping processes are not taken into account.

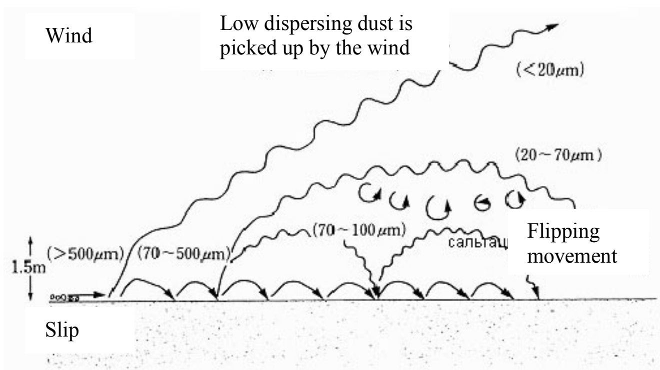

Fig. 1. Particle trajectories depending on their size, adopted from (Pye 1987).

2.1. Analytical Model

In the majority of models of pollution, spreading lies unsteady turbulent diffusion equation. Under repeated indices, we assume summation according to (Nistadta, Van Dopa 1985):

$$\frac{\partial C}{\partial t} = K_i \frac{\partial^2 C}{\partial x_i^2} - V_i \frac{\partial C}{\partial x_i} \qquad (1)$$

Where C - concentration of pollutants, K_i - turbulent diffusion coefficient, V_i - the wind velocity. It is assumed that the turbulent diffusion coefficients do not depend on coordinates, and time.

Secondary mass transfer can be represented as the work of instant point of source pollution. Then the analytical solution of equation (1) is represented as:

$$C(x_1, x_2, x_3, t) = Q \cdot G(x_1, x_2, x_3, t) \qquad (2)$$

Where $G(x_1, x_2, x_3, t)$ is Green's function (Kartashov 1985). For the one-dimensional case the Green's function is as follows:

$$G(x_1, t) = \exp\left(-\frac{[(x_1 - x_1^0) - v_1 t]^2}{4K_1 t}\right) / (2\sqrt{\pi K_1 t}) \qquad (3)$$

According to the formulas, we can calculate the concentrations of the pollutant at any moment *t*.

To describe the distribution of contaminants from a continuous point source of constant power can be used Setton equation (Berlyand 1985). Formula of Setton-dimensional case can be obtained as a stationary solution of equation (1):

$$C(x) = \frac{Q}{\sigma_x \sqrt{2\pi}} \exp\left(-\frac{(x - x_0)^2}{2\sigma_x^2}\right) \qquad (4)$$

Where σ_x - dispersion coefficient, x_0 - source position, Q - source power.

2.2. Cellular automations

In computing environment, cellular automation all the processes are considered in a discrete space - n-dimensional grid, where each cell is a part of the simulated space. The interaction of particles is described by the rules of the pollutant CA united throughout the space, and determines the state of a given cell, depending on the model given in stochastic processes and the state of the neighboring cells. Long-range rules are limited to select a neighborhood (of neighbor cells).

The unit of length is the cell and the unit of time - one iteration cycle. Explores the changing state of the system in time. Over time step (iteration), all cells CA change their state in accordance with the rules of CA. In this way, we obtain a complex dynamic self-developing system.

This approach allows you to get many individual models to establish the fields of surface contamination by simply combining individual CA rules and change the values of the control parameters corresponding to the characteristics of the real physical and chemical processes. The calculation results are probabilistic in nature - for the same model with the same conditions will be obtained various fields of pollution, coinciding "on average".

2.3. Model description of wind transfer using CA rules

The symbols: **S** – state of the cell "source of pollution", **F –** cell in a state of "pollutant, soaring in the atmosphere" **E** – cell in the "environment, **F' –** cell in a "contaminant dropped out on the surface" », M_{ij} – neighborhood of the cell (i, j), $X_{i,j}(t)$ – state of the cell (i, j) at the moment of time t:

$M_{ij} = \{X_{i-1,j+1}; X_{i-1,j}; X_{i-1,j-1}; X_{i,j+1}; X_{i,j-1}; X_{i+1,j+1}; X_{i+1,j}; X_{i+1,j-1}\}$

2.4. Rules of the digital simulation model

<u>Rule 1</u>. Emission of air pollutants:

$X_{i,j}(t) \in E \rightarrow |X_{i,j}(t+1) \in F$ with probability pF , if $\{M_{i,j} \cap S \neq \varnothing\}$

<u>Rule 2</u>. The wind mass transfer:

Xi,j(t) ∈ E → | Xi,j(t+1) ∈ F with probability pVF($\vec{V}$), if { Mi,j∩F ≠ ∅};

state transition probability in this case depends on the wind speed and direction $\vec{V}$.

Rule 3. Deposition:

Xi,j(t) ∈ F → |Xi,j(t+1) ∈ F' with probability p'F;

state transition probability in this case depends on the mass of the particle.

Rule 4. Turbulent diffusion:

Xi,j(t) ∈ E → | Xi,j(t+1) ∈ F with probability pTF, if { Mi,j∩F ≠ ∅};

For computer calculations, these rules are encoded in a universal laboratory PyCALab, written in the language of python (Medvedeva 2006, Gubarev 2007).

3. THE WIND MASS TRANSFER POLLUTION FROM A LINE SOURCE: A COMPUTER EXPERIMENT AND ANALYTICAL MODEL

In the model, homogeneous initial and boundary conditions were laid. Modeling happened on the grid size 70x20 cell with one line source pollution constant intensity. The duration of each computer simulation (calculation of the field of pollution) amounted to 50,000 iterations. As a real analogue of the pollutant in the model was chosen the dust and was dropped from the model of the physical and chemical processes in the atmosphere. The spread of pollutants carried by the wind and turbulent diffusion. Recording CA rules in the laboratory PyCALab as follows:

Emission – rule 1

("rule", "emition_solid_part", ("simple", 1)),

The wind mass transfer – rule 2

("rule", "directional_diffusion_one_type", ("simple")),

Turbulent diffusion – rule 4

("rule", "random_diffusion_one_type", ("simple", 0.1)),

Deposition – rule 3

("rule", "falling_solid_part", ("simple", 0.007)),

The simulation results are shown in Fig. 2-4.

There is an abrupt change in the concentrations of the pollutant in the neighboring points of the profile (up to 25% of the absolute value) in the apparent decrease monotonically trend with distance from the source. These jumps are the result of stochastic processes of wind mass transfer. Detection of significant inhomogeneity of the field surface contamination is in good agreement with the experimental data of snow survey - study of the dust accumulated in snow cover during the winter period. It was experimentally proved by (Chukanov 2006) that the differences in the weight of the dust collected on spots of 314 cm^2 and at a distance of 5 cm from each other could be up to 40%. The decrease in the mass of dust that fell away from the emission source is not monotonous and spasmodic character.

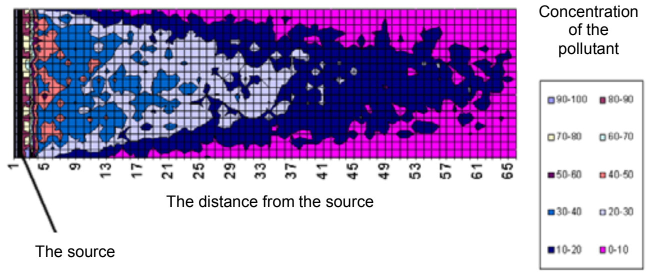

Fig. 2. Model field of pollution from line source of constant power (using the rules of emission, of wind transfer, turbulent diffusion and deposition).

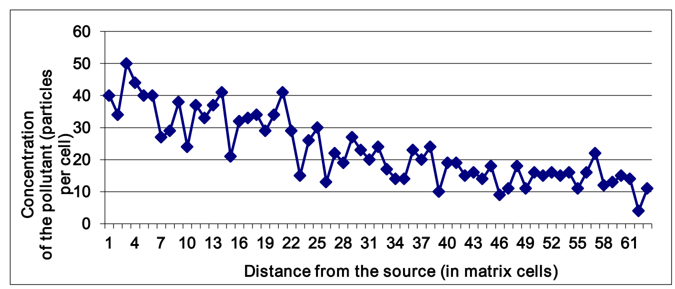

Fig. 3. Central profile of the pollution field shown in Fig. 2.

When averaging the values of pollutant concentration along the central profile on the computer implementation of twenty fields of surface contamination resulting curve becomes smoother, Fig. 4, and is close to the analytical solution of the equation Setton (4) for the one-dimensional case.

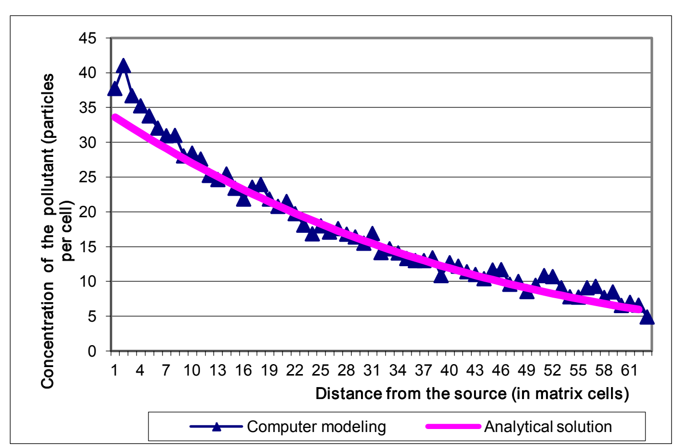

Fig. 4. Averaging over the ensemble, 20 computer implementations. Analytical solution of Setton equation (4) is obtained at values of $\sigma_x = 80 CellUnits$, $x_0 = -150 CellUnits$, $Q = 4 \cdot 10^4\ particles / cell^3$.

Thus, the comparison of the results of calculations of the wind dust mass transfer by cellular automation and solutions of differential equations shows that they are in good agreement. Differential equations give the averaged, while the settlement of CA simulation model can detect the statistical features of the distribution of concentrations of specific contaminants field.

4. CONCLUSION

This work provides a brief description of the two models of wind mass transfer - analytical and numerical simulation - and performed calculations for one-dimensional case. A feature of the results of calculations for the analytical model is smooth (averaged) dependence of the concentration of pollutants on the distance from the source. A feature of the results of calculations by the second - a simulation model in the computing environment of cellular automata - is "noisy" due to the dependence of random nature of the mass transfer in a particular realization (settlement computer experiment). An abrupt change in the concentrations of the pollutant in the neighboring points, sometimes as high as 25% in the apparent trend decreases monotonically with distance from the source, which is in good agreement with the experimental data of snow survey: the intensity distribution loss particulate pollutant has very nonmonotonic at short distances.

It is shown that the average concentration of the pollutant in many computer implementations of the field of surface contamination becomes smoother and closer to a decision on the analytical model. The results of this study demonstrated that for the correct reconstruction of fields of surface contamination on the values of concentrations of pollutants in selected areas on the samples should be carried out with the assistance of mathematical models of different types - both analytical (differential equations) and numerical simulation (cellular automata), depending on features of tasks. Some mentioned above features of simulation model make it more preferable for pollution forecast calculations for optimal control purpose.

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REFERENCES

Beklemishev K.A. (2006). Universal laboratory of cellular automata PyCAlab. *Bull. of Ural State Tech. Univ*. № 6, p. 117-122. (in Russian)

Berg D.B., Beklemishev K.A., Sergeev A.P., Medvedeva M.A. (2005). Program complex for surface contamination simulation. Russian patent office certificate for computer program №2005612986.

Berlyand M.E. (1985). *Prediction and control of atmospheric pollution*. Leningrad: Gidrometeoizdat (in Russian)

Chukanov V.N, Sergeev A.P, Ovchinnikov S.M, Medvedev A.N. (2006). Diagnostics of Snow-Cower Contamination with Soluble and Insoluble Metal Impurities. *Russian Journal of Nondestructive Testing,* Vol. 42, № 9. pp. 630-636.

Gubarev S.V., Beklemishev K.A., Berg D.B. (2007). Simulation of two-phase distribution of air pollution. *Proc. Int. Youth Sci. Conf*. Yerevan, Armenia Republic, pp 22-27. (in Russian)

Kartashov EM (1985). *Analytical methods in the theory of thermal conductivity of solids*. Moscow: Higher School, 480 p. (in Russian)

Medvedeva M.A., Sergeev A.P., Beklemishev K.A., Berg D.B. (2006). Simulation of surface contamination space distribution *Conf. proc. "Information and mathematical approach to economy, technology and education"*. Ekaterinburg, P. 1, pp. 62-66. . (in Russian)

Toffoli Toffoli T., Margolus N. (1991). *Cellular automata machines*. Moscow: Mir. 280 pp.

Pye K. (1987): *Aerolian Dust and Dust Deposits*. Academic Press, p. 49

Nistadta F.T., Van Dopa M. H. (eds) (1985). *Atmospheric turbulence and modeling of impurities*. Leningrad: Gidrometeoizdat, 351 p.